4-Cyclohexylphenylacetic acid 35889-00-0 | DTXSID60189446

Model Performance

Model	Data	
Model	Dala	

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)		
Q2	RMSE	R2	RMSE	R2	RMSE	
0.85	0.69	0.86	0.67	0.86	0.78	

Model Results

Predicted value: 3.90

Global applicability domain: Inside

Local applicability domain index: 6.59e-01

Confidence level: 7.58e-01

Nearest Neighbors from the Training Set

Image not found

Ibuprofen
Measured: 3.97
Predicted: 3.66

Image not found

4-Cyclohexylphenylacetic acid

Measured: 3.91 **Predicted:** 3.90

Image not found

6-Chlorothymol Measured: 3.92 Predicted: 3.48